Coherence, Multiple Scattering and Scaling in Diffractive Imaging

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Diffractive imaging allows the formation of new kinds of images, not possible with a conventional microscope. Since one has access to the complex wavefield, a dark-field image may be formed which is linear in the charge-density (for X-rays) or electrostatic potential (electrons). The physical introduction of a beamstop in conventional microsopy produces non-linear dark-field images containing artifacts such as maxima where either minima or maxima in density occur in the sample.

An arrangement in which the X-ray source is conjugate to the sample may have advantages, and will produce partially coherent illumination if the source is extended. We analyse the degree of coherence in this case, where the effect is equivalent to lateral translation of the sample. We also show that for the case where the source is conjugate to the detector, the coherence patch for diffractive imaging must be larger than the object, corresponding to the requirement that the beam-divergence must be less than the oversampling angle (for critical Shannon sampling of the diffracted intensity). This has implications for exposure time calculations.

In the early days of LEED theory it was thought that absorption effects might be more severe than multiple elastic scattering. In that case, the ratio of the strength of the two effects is controlled by a complex optical potential, and this ratio does not depend on beam energy. For X-rays, where it does, the question arises as to how the relative importance of the two effects varies across an absorption edge, and whether beam energies may therefore be found where the attentuation length (due to photoelecton production) is much less than the multiple scattering extinction distance. Soft-Xray multislice calculations will be used to investigate this question.

If time allows, a new application of the iterative Ozlayni filipping algorithm (a HiO relative) to powder X-ray diffraction data will be shown to have advantages. (Wu et al, Nature Materials, 5, 647 (2006)). The dependance of exposure time on beam energy and on resolution for the Serial Crystallography scheme may also be reviewed. This scheme sprays hydrated, laser-aligned proteins in single-file across the ALS synchrotron in order to determine their structure (Starodub et al , J. Chem Phys. 123, 244304 (2005)) . Supported by ARO and NSF.